

Confinement of electrons in layered metals

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(February 1, 2008)

We analyze the out of plane hopping in models of layered systems where the in-plane properties deviate from Landau's theory of a Fermi liquid. We show that the hopping term acquires a non trivial energy dependence, due to the coupling to in plane excitations, and can be either relevant or irrelevant at low energies or temperatures. The latter is always the case if the Fermi level lies close to a saddle point in the dispersion relation.

Layered materials have been object of intensive study since they present important physics. Unusual properties are derived from the anisotropy and periodicity along the axis perpendicular to the planes [1]. Among the most studied layered materials are the high-temperature cuprate superconductors. These compounds present a strong anisotropy and are treated as two-dimensional systems in many approaches. In the normal state the transport properties within the CuO₂ planes are very different from those along the c-axis: electron motion in the c-direction is incoherent in contrast with the metallic behavior of the in-plane electrons as probed by the different ρ_c and ρ_{ab} resistivities and their different dependence with temperature [2,3]. Optical conductivity measurements confirm the anomalous c-axis properties [4]. The relevance of the nature of the conductance in the direction perpendicular to the CuO₂ planes to the nature of the superconducting phase has been remarked on both theoretical [5–7] and experimental [8] grounds. The anomalous nature of the out of plane properties in the cuprates, and in analogy with the one dimensional Luttinger liquid, has led to the proposal of the failure of the conventional Fermi-liquid theory in these compounds [5]. An alternative explanation of the emergence of incoherent behavior in the out of plane direction has been proposed in terms of the coupling of the interlayer electronic motion to charge excitations of the system [7]. This approach implicitly assumes that electron-electron interactions modify the in-plane electron propagators in a non trivial way, at least at distances shorter than the elastic mean free path, l . The strong angular dependence of both the scattering rate and the interplane tunneling element can also lead to the observed anisotropies [9].

Graphite, another layered material, presents a in-traplane hopping much larger than the interplane hybridization. The unconventional transport properties of graphite such as the linear increase with energy of the inverse lifetime [10] (see also [11]), suggest deviations from the conventional Fermi liquid behavior, which could be due to strong Coulomb interactions unscreened because of the lack of states at the Fermi level [12].

In the following, we extend the methods used in [7] to the clean limit, $l \rightarrow \infty$, and show that, for certain models of correlated electrons [12,13] the interplane hopping between extended states can be a relevant or an irrelevant variable, in the RG sense, depending on the strength of the coupling constant. The scheme used here is based on the renormalization group analysis as applied to models of interacting electrons [14,15]. For the problem of inter-chain hopping between Luttinger liquids, it recovers well known results [16–18].

We first present the method of calculation, and show the results it gives in one dimension. Then, we apply it to two dimensional models which show deviations from FL behavior. The main physical consequences of our calculation are discussed in the last section.

The method of calculation. In the presence of electron-electron interactions, tunneling processes are modified by inelastic scattering events. If the excitations of the systems (electron-hole pairs, plasmons) are modelled as bosonic modes, one can write an effective electron-boson hamiltonian of the type:

$$\mathcal{H}_{e-b} = \sum \mathbf{t}_{ij} c_i^\dagger c_j + \sum \omega_k b_k^\dagger b_k + \sum g_{k,i} c_i^\dagger c_i (b_k^\dagger + b_k) \quad (1)$$

where the \mathbf{t}_{ij} describe the electronic hopping processes. The electron-boson interaction leads to a Franck Condon factor which reduces the effective tunneling rate. The electron propagators acquire an anomalous time, or energy, dependence:

$$\langle c_i^\dagger(t) c_j(t') \rangle \sim \frac{C_{ij}}{t - t'} \times \exp \left\{ \int d\omega \left[1 - e^{i\omega(t-t')} \right] \frac{J_{ij}(\omega)}{\omega^2} \right\} \quad (2)$$

where:

$$J_{ij}(\omega) = \sum_k |g_{ik} g_{jk}|^2 \delta(\omega - \omega_k) \quad (3)$$

This expression can be generalized, taking into account the spatial structure of the coupling to:

$$\begin{aligned} \langle \Psi_i^\dagger(t) \Psi_j(t') \rangle &\sim \frac{C_{ij}}{t-t'} \times \\ &\times \exp \left\{ \int_{\vec{k}} \int_{\Omega} \int_{\Omega} d^2 \vec{r} d^2 \vec{r}' d^2 \vec{k} e^{i \vec{k}(\vec{r}-\vec{r}')} \right. \\ &\left. \int d\omega \left[1 - e^{i\omega(t-t')} \right] \frac{V_{eff}(\vec{k}, \omega)}{\omega^2} \right\} \quad (4) \end{aligned}$$

where Ω is the region of overlap of the wavefunctions $\Psi_i(\vec{r})$ and $\Psi_j(\vec{r})$. This expression, which can be seen as the exponential of the leading frequency dependent self-energy correction to the electron propagator, has been extensively used in studies of tunneling in zero dimensional systems (single electron transistors) which show Coulomb blockade [19], one dimensional conductors [20], and disordered systems in arbitrary dimensions [21].

The effective interaction can, in turn, be written in terms of the response function as:

$$V_{eff}(\vec{k}, \omega) = V^2(\mathbf{k}) \text{Im} \chi(\vec{k}, \omega) \quad (5)$$

In a Fermi liquid, we have $V_{eff}(\vec{k}, \omega) \approx \alpha(\vec{k})|\omega|$ for $\omega \ll E_F$, where E_F is the Fermi energy, so that:

$$\begin{aligned} \lim_{(t-t') \rightarrow \infty} \langle \Psi^\dagger(t) \Psi(t') \rangle &\sim \frac{1}{(t-t')^{1+\bar{\alpha}}} \\ \bar{\alpha} &= \int_{\vec{k}} \int_{\Omega} \int_{\Omega} d^2 \vec{r} d^2 \vec{r}' d^2 \vec{k} e^{i \vec{k}(\vec{r}-\vec{r}')} \alpha(\vec{k}) \quad (6) \end{aligned}$$

The parameter $\bar{\alpha}$ gives the correction to the scaling properties of the Green's functions. It is easy to show that, in an isotropic Fermi liquid in D dimensions, $\lim_{l \rightarrow \infty} \bar{\alpha} \propto l^{1-D}$, where l is the linear dimension of the (localized) electronic wavefunctions $\Psi(\vec{r})$. This result is due to the dependence on \vec{k} of the response functions, as $\text{Im} \chi(\vec{k}, \omega) \sim |\omega|/(k_F^{D-1}|\vec{k}|)$. Thus, for $D > 1$, we recover coherent tunneling in the limit of delocalized wavefunctions.

In one dimension, one can use the non interacting expression for $\text{Im} \chi_0(\vec{k}, \omega)$, to obtain:

$$\begin{aligned} &\int d^2 \vec{r} d^2 \vec{r}' d^2 \vec{k} e^{i \vec{k}(\vec{r}-\vec{r}')} \int d\omega \left[1 - e^{i\omega(t-t')} \right] \frac{V_{eff}(\vec{k}, \omega)}{\omega^2} \\ &\propto \left(\frac{U}{E_F} \right)^2 \times \begin{cases} 0 & t-t' \ll l/v_F \\ \log[v_F(t-t')/l] & t-t' \gg l/v_F \end{cases} \quad (7) \end{aligned}$$

where we have assumed a short range interaction, U . Hence, the Green's functions have a non trivial power dependence on time, even in the $l \rightarrow \infty$ limit, in agreement with well known results for Luttinger liquids [20]. In order to obtain the energy dependence of the effective tunneling between \vec{k} states near the Fermi surface, one needs to perform an additional integration over $d\vec{r}$. In general, near a scale invariant fixed point, $\omega \propto |\vec{k}|^z$, and for a 1D conductor one knows that $z = 1$. Hence, $\text{Im} G(\omega, k_F) \propto \omega^{-z+\bar{\alpha}} \sim \omega^{-1+\bar{\alpha}}$. The flow of the hopping

terms under a Renormalization Group scaling of the cut-off is [18]:

$$\Lambda \frac{\partial(\mathbf{t}/\Lambda)}{\partial \Lambda} = \begin{cases} -\bar{\alpha} & \text{localized hopping} \\ 1 - \bar{\alpha} & \text{extended hopping} \end{cases} \quad (8)$$

where \mathbf{t} denotes a hopping term, between localized or extended states. In the latter case, the hopping becomes an irrelevant variable [16] for $\bar{\alpha} > 1$.

Graphene planes. The simplest two dimensional model for interacting electrons where it can be rigorously shown that the couplings acquire logarithmic corrections in perturbation theory is a system of Dirac fermions ($\epsilon_k = v_F |\vec{k}|$), with Coulomb, $1/|\vec{r} - \vec{r}'|$, interaction. This model can be used to describe isolated graphene planes [12], and can help to understand the anomalous behavior of graphite observed in recent experiments [10, 11].

In order to apply the procedure outlined in the previous section, one needs the Fourier transform of the interaction, $e^2/(\epsilon_0 |\vec{k}|)$, where e is the electronic charge, and ϵ_0 is the dielectric constant, and the susceptibility of the electron gas. For a single graphene plane, this quantity is:

$$\chi_0(\vec{k}, \omega) = \frac{1}{8} \frac{|\vec{k}|^2}{\sqrt{v_F^2 |\vec{k}|^2 - \omega^2}} \quad (9)$$

These expressions need to be inserted in equations (5) and (4). Alternatively, we can use the RPA, and include the effects of interplane screening:

$$\chi_{RPA}(\vec{k}, \omega) = \frac{\sinh(|\vec{k}|d)}{\sqrt{[\cosh(|\vec{k}|d) + \frac{2\pi e^2}{\epsilon_0 |\vec{k}|} \sinh(|\vec{k}|d) \chi_0(\vec{k}, \omega)]^2 - 1}} \quad (10)$$

where d is the interplane spacing. The imaginary part, $\text{Im} \chi_0(\vec{k}, \omega)$, is different from zero if $\omega > v_F |\vec{k}|$.

For simplicity, we consider the expression in eq.(9), as it allows us to obtain analytical expressions. We cut off the spatial integrals at a scale, l , of the order of the electronic wavefunctions involved in the tunneling. We obtain an expression similar to that in eq.(7) except that the prefactor $(U/E_F)^2$ is replaced by $e^4/(\epsilon_0 v_F)^2$. Thus, the propagators acquire an anomalous dimension. As in 1D, the value of the exponent z which relates length and time scales is $z = 1$. The scaling of the hoppings now are:

$$\Lambda \frac{\partial(\mathbf{t}/\Lambda)}{\partial \Lambda} = \begin{cases} -1 - \bar{\alpha} & \text{localized hopping} \\ 1 - \bar{\alpha} & \text{extended hopping} \end{cases} \quad (11)$$

The extra constant in the first equation with respect to eq. (8) reflects the vanishing of the density of states at the Fermi level for two dimensional electrons with a Dirac dispersion relation.

In graphite, the dimensionless coupling constant, e^2/v_F , is of order unity. Under renormalization, it flows

towards zero [12]. Thus, interplane tunneling is a relevant variable, although, in a dirty system with a finite mean free path, interplane tunneling can become irrelevant [22].

Saddle point in the density of states. The Fermi surface of most hole-doped cuprates is close to a Van Hove singularity [23]. The possible relevance of this fact to the superconducting transition as well as to the anomalous behavior of the normal state was put forward in the early times of the cuprates and gave rise to the so-called Van Hove scenario [24].

We shall apply the mechanism described in section II to study the interlayer hopping of two electronic systems described by the $\mathbf{t}-\mathbf{t}'$ Hubbard model and whose Fermi surface lies close to a Van Hove singularity.

The $\mathbf{t}-\mathbf{t}'$ -Hubbard model has the dispersion relation

$$\varepsilon(\vec{\mathbf{k}}) = -2\mathbf{t} [\cos(k_x a) + \cos(k_y a)] - 2\mathbf{t}' \cos(k_x a) \cos(k_y a) , \quad (12)$$

This dispersion relation has two inequivalent saddle points at A $(\pi, 0)$ and B $(0, \pi)$. The Van Hove model in its simplest formulation is obtained by assuming that for fillings such that the Fermi line lies close to the singularities, the majority of states participating in the interactions will come from regions in the vicinity of the saddle points [25]. Taylor expanding eq. (12) around the two points gives the effective relation

$$\varepsilon_{A,B}(\vec{\mathbf{k}}) \approx \mp(\mathbf{t} \mp 2\mathbf{t}')k_x^2 \pm (\mathbf{t} \pm 2\mathbf{t}')k_y^2 , \quad (13)$$

which leads to the effective hamiltonian:

$$\mathcal{H} = \sum_{i=1,2;k,s}^{\varepsilon_{i,k} < \Lambda_0} \varepsilon_{i,k} c_{k,i,s}^\dagger c_{i,k,s} + \sum u_{i,i';s,s'} c_{i,k,s}^\dagger c_{i',k',s'} c_{i'',k'',s''}^\dagger c_{i''',k''',s'''} , \quad (14)$$

where Λ_0 is a high energy cutoff which sets the limit of validity of the effective description. The particle-hole susceptibility has been computed in [13]:

$$\text{Im } \chi(\vec{\mathbf{k}}, \omega) = \frac{1}{4\pi\varepsilon(\vec{\mathbf{k}})} \left(\left| \omega + \varepsilon(\vec{\mathbf{k}}) \right| - \left| \omega - \varepsilon(\vec{\mathbf{k}}) \right| \right) , \quad (15)$$

where $\varepsilon(\vec{\mathbf{k}})$ is the dispersion relation (13).

The long time dependence of the Green's function is determined by the low energy behavior of χ :

$$\lim_{\omega \rightarrow 0} \text{Im } \chi(\vec{\mathbf{k}}, \omega) \sim \frac{\omega}{\varepsilon(\vec{\mathbf{k}})}$$

Inserting this expression in eqs.(4) and (5), we can see that, irrespective of the details of the interaction, in the presence of a Van Hove singularity the exponent $\bar{\alpha}$ in the time dependence of the Green's function goes as:

$$\lim_{\Omega \rightarrow \infty} \bar{\alpha} \propto \log(l) ,$$

where l , as before, is the length scale which characterizes the wavefunction of the tunneling electron, and $\Omega \propto l^2$ is the size of the integration region in eq.(4).

The details of the anomalous dimension of the propagator in this case depend on the nature of the interactions which determine $V_{eff}(\vec{\mathbf{k}}, \omega) = V^2(\vec{\mathbf{k}}) \text{Im} \chi(\vec{\mathbf{k}}, \omega)$. To make contact with previous works [7], we have computed the parameter $\bar{\alpha}$ for different possible interactions:

a) Unscreened Coulomb potential, $V(\vec{\mathbf{k}}) = \frac{2\pi e^2}{\epsilon_0 |\vec{\mathbf{k}}|}$. Due to the highly singular interaction, the ω dependence of the effective potential is not linear and $\bar{\alpha}$ is not well defined. The effective potential eq. (5) is computed to be:

$$V_{eff}(\vec{\mathbf{k}}, \omega) = \frac{e^4}{\epsilon_0^2 \mathbf{t}} \left[1 + \log \left(\frac{\omega}{\omega_0} \right) \right]$$

where $\omega_0 = |E_F - E_{VH}|$ is a low-energy cutoff, required to avoid divergences in the integrals. The Fermi energy is E_F and the position of the saddle point is at E_{VH} .

b) Screened interaction of the Hubbard type, $V(\vec{\mathbf{k}}) = Ua^2$, where a is the lattice unit.

$$\bar{\alpha} = \frac{4U^2}{\pi \mathbf{t}^2} \frac{1}{(2\pi)^2} K_M \left[1 + \frac{1}{2} \log \left(\frac{\Lambda}{\omega} \right) \right] ,$$

where Λ is a high-energy cutoff, and

$$K_M = \frac{1}{2} \log \left| \frac{k_x + k_y}{k_x - k_y} \right| ,$$

where $k_x, k_y \sim \sqrt{\omega_0}$.

c) Thomas-Fermi screened potential,

$$V(\vec{\mathbf{k}})^2 = \frac{(2\pi e^2)^2}{\epsilon_0^2 (k^2 + k_{FT}^2)} , \quad \bar{\alpha} \sim \frac{2e^4 k_{FT}^2}{\epsilon_0 \pi \mathbf{t}^2} \log^2(k_{FT}/k) ,$$

where k_{FT} is the Fermi-Thomas wavevector, and, as before, $k \sim \sqrt{\omega_0}$. This is an intermediate situation between the two previous cases.

Finally, in the case of a layered system, we can use the RPA summation, including interlayer interactions, eq.(10). In this case, $z = 2$, and the scaling equations for the hoppings are the same as in eq.(8).

A numerical computation provides the effective potential shown in fig. [1].

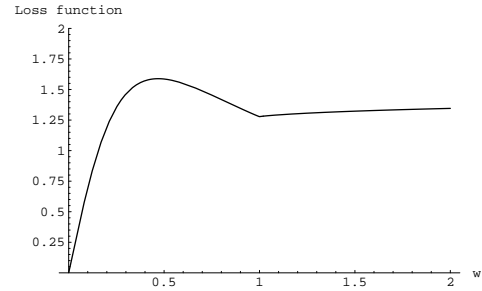


FIG. 1. Effective potential eq. (5) as a function of the energy for fixed $\vec{\mathbf{k}}$ for a system of Van Hove layers coupled by Coulomb interaction .

Fig. [1] compares well with the experimental plots of the loss function given in [26], what reveals that the Van Hove model is also compatible with transport experiments. The results for the parameter $\bar{\alpha}$ extracted from the numerical computation are in qualitative agreement with the analytical expressions given in cases b) and c) above.

In all cases $\bar{\alpha}$ diverges as $E_F \rightarrow E_{VH}$. Thus, interlayer hopping is an irrelevant variable, and scales towards zero as the temperature or frequency is decreased. This additional logarithmic dependence can be seen as a manifestation of the \log^2 divergences which arise in the treatment of this model [13]. Note that, as in the graphene case, the coupling constants are also energy dependent, and grow at low energies, suppressing even further the interlayer tunneling.

Conclusions. We have discussed the suppression of interlayer tunneling by inelastic processes in two dimensional systems in the clean limit. Our results suggest that, when perturbation theory for the in-plane interactions leads to logarithmic divergences, the out of plane tunneling acquires a non trivial energy dependence. This anomalous scaling of the interlayer hopping can make it irrelevant, at low energies, if the in-plane interactions are sufficiently strong. This is always the case if the Fermi level of the interacting electrons lies at a van Hove singularity (note that the Fermi level can, in certain circumstances, be pinned to the singularity [13]). Thus, we have shown that insulating behavior in the out of plane direction is not incompatible with gapless in-plane properties.

Acknowledgements. We are thankful to R. Markiewicz for a careful reading of the manuscript. The financial support of the CICyT (Spain), through grants no. PB96-0875, 1FD97-1358 and BFM2000-1107, is gratefully acknowledged.

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